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Author(s): Cheng Liu, MST-8, LANL

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On the Minimum Size of Representative Volume Element (RVE)

C. LIU
Materials Science & Technology Division, Los Alamos National Laboratory
Los Alamos, New Mexico 87545, USA

Abstract

In this investigation, the minimum size of the representative volume element (RVE) of a heterogeneous material is determined experimentally using the digital image correlation (DIC) technique. Experiments of uniaxial compression and thermal expansion were conducted on the PBS 9501, a high explosive simulant material. The minimum size of the representative volume element (RVE) of the PBS 9501 heterogeneous material, where the average crystal diameter of the material is on the order of 100 μm, was determined to be approximately 1.5 mm. This result is consistent with those numerical calculations on polycrystalline materials and some other composites.

1 Introduction

Almost all the engineering materials are heterogeneous in nature. They are either compounds composed of several different phases or aggregates of crystals with different sizes and orientations. Theoretical estimation of the macroscopic and overall constitutive behavior of the heterogeneous material plays a central role in many engineering applications. Such theoretical estimates are usually obtained by homogenization processes. At the heart of the homogenization process is the so-called representative volume element, or RVE. In order for the constitutive models, based on the homogenization approach, to accurately describe the overall response of the heterogeneous solids, the minimum size of the representative volume element must be known.

Hill [1] gave the first definition for the representative volume element and later he proposed a more descriptive definition for the RVE that involves a very detailed calculation [2]. To perform Hill's calculation requires a very detailed description of the microstructure within the element. Drugan and Willis [3] adopted an alternative definition for the RVE. They regard a RVE as the smallest material volume element of the heterogeneous solid for which the usual spatially constant "overall modulus" macroscopic constitutive representation is a sufficiently accurate model to represent mean constitutive response. Drugan and Willis [3] studied the minimum RVE size of an elastic composite composed of a random dispersion of non-overlapping identical spheres. Gusev [4] investigated the same problem but by using numerical technique. For any realistic heterogeneous material with a random microstructure, determining the minimum size of the RVE remains an open question.

In this study, we carried out experimental investigation to study the nature of heterogeneity and to determine the minimum RVE size of a heterogeneous material, PBS 9501, a high explosive simulant material. Two different experiments were conducted. One was uniaxial compression, where an overall uniform deformation is applied to the sample, the other was thermal expansion of the sample subjected to slow heating. Using the digital image correlation (DIC) technique, we were able to measure the strain field under a fixed externally applied load or a given temperature rise. The results of our measurement depend on the material element size used in the digital image correlation calculation. We found that when the material element exceeds a certain size, the mean value of the distribution of strain converged to a constant. Meanwhile, the scatter of strain data becomes smaller when the material element size increases. By examining the variation of the mean value of strain, as a function of the material element size, the minimum size of the RVE for PBS 9501 simulant was determined. Implications of these observations and measurements will be discussed.

2 Digital Image Correlation (DIC) Technique

Digital image correlation technique relies on the computer vision approach to extract the whole-field displacement data, that is, by comparing the features in a pair of digital images of a specimen surface before and after deformation. Since a feature in the digital image correlation technique (DIC) was explored in our experimental study, a brief description of the underlying principle of the DIC technique is given below.

Consider a planar object illuminated by a light source and suppose that the object undergoes planar deformation. Let $\mathbb{R}$ be a small region of the undeformed two-dimensional object and $\mathbb{R}_*$ be the same region but in the deformed configuration. The light intensity pattern of the undeformed region $\mathbb{R}$ is denoted by $I(\boldsymbol{x})$ where $\boldsymbol{x} \in \mathbb{R}$, while the light intensity pattern of the deformed region $\mathbb{R}_*$ is denoted as $I_*(\boldsymbol{y})$ where $\boldsymbol{y} \in \mathbb{R}_*$ and $\boldsymbol{y} = \hat{\boldsymbol{y}}(\boldsymbol{x})$. Both $I(\boldsymbol{x})$ and $I_*(\boldsymbol{y})$ are assumed to be in unique and one-on-one correspondence with the respective object surface, and they are integer-valued functions ranging from 0 to 255 for an 8-bit gray scale digital camera. If during the deformation process of the small region, the intensity pattern only deforms but does not alter its local value, then we should have

$$I_*(\boldsymbol{y}) = I_*(\hat{\boldsymbol{y}}(\boldsymbol{x})) = I(\boldsymbol{x}), \quad \forall\, \boldsymbol{x} \in \mathbb{R}. \tag{1}$$

As a result, the measurement of the displacement field using the digital image correlation technique can be formulated into the following mathematical problem: *By knowing the two intensity patterns $I(\boldsymbol{x})$ and $I_*(\boldsymbol{y})$ of the same region before and after deformation, find a mapping relation $\boldsymbol{y} = \hat{\boldsymbol{y}}(\boldsymbol{x})$ such that*

$$I_*(\hat{\boldsymbol{y}}(\boldsymbol{x})) - I(\boldsymbol{x}) = 0, \quad \forall\, \boldsymbol{x} \in \mathbb{R}. \tag{2}$$

Furthermore, if the deformation is *homogeneous*, i.e., if the deformation is such that

$$\hat{\boldsymbol{y}}(\boldsymbol{x}) = \boldsymbol{F}\boldsymbol{x} + \boldsymbol{b}, \quad \boldsymbol{x} \in \mathbb{R}, \tag{3}$$

where $\boldsymbol{F}$ is a constant tensor and $\boldsymbol{b}$ is a constant vector, and for two-dimensional deformation, the components of $\boldsymbol{F}$ and $\boldsymbol{b}$ in an orthonormal coordinate system can be written as

$$[F_{\alpha\beta}] = \begin{bmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{bmatrix}, \quad [b_\alpha] = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \tag{4}$$

the above mathematical problem becomes to find a tensor $\boldsymbol{F}$ with four scalar components, and a vector $\boldsymbol{b}$ with two components, such that

$$I_*(\boldsymbol{F}\boldsymbol{x} + \boldsymbol{b}) - I(\boldsymbol{x}) = 0, \quad \forall\, \boldsymbol{x} \in \mathbb{R}, \tag{5}$$

with the restriction of $\det \boldsymbol{F} = f_{11} f_{22} - f_{12} f_{21} > 0$. The Lagrangian strain tensor $\boldsymbol{E}$ (also called Green-Lagrangian strain tensor) can be calculated by

$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^\top \boldsymbol{F} - \boldsymbol{I}), \tag{6}$$

where $\boldsymbol{I}$ is the identity tensor. Detailed descriptions regarding the DIC technique can be found in [5, 6, 7].

Note that any general deformation can always be viewed as locally homogeneous provided that the region $\mathbb{R}$ to be considered is sufficiently small. On the other hand, for any given size of the material element $\mathbb{R}$, the strain measurement obtained through the digital image correlation, as given in Eq.(6), represents an average strain that the material element $\mathbb{R}$ is experiencing. Now consider a sample element made of a heterogeneous material and the element is subjected to the boundary condition $u_i = \epsilon_{ij} x_j$, where u_i is the displacement, x_i is position, and ϵ_{ij} is the strain tensor within the element if it is made of a homogeneous material. Suppose that we are measuring the strain field within the sample element using the digital image correlation technique described above. When the size of the material element $\mathbb{R}$ used in the calculation is small, one would expect that the measured average strain of the element $\mathbb{R}$ is different from ϵ_{ij} due to the heterogeneous nature of the material. Only when the size of the material element $\mathbb{R}$ becomes sufficiently large, the measured average strain of the element $\mathbb{R}$ will approach the applied strain ϵ_{ij}. By examining the variation of the measured average strain of the element $\mathbb{R}$ as a function of the size of the element $\mathbb{R}$, the minimum size of the representative volume element (RVE) of the tested heterogeneous material can be determined. Similar concept was also employed by Ren and Zheng [8] in their numerical study of the minimum sizes of representative volume elements of cubic polycrystals by monitoring the variation of the nominal modulus tensor as a function of the size of a finite volume.

3 Material Preparation

A high explosive simulant material, referred to as PBS 9501, was used in the present investigation. The reason of choosing such a material is that PBS 9501 can simulate, at the macroscopic level, the mechanical behavior of the

PBX 9501 high explosive, which is composed by the HMX energetic crystal and a polymeric binder, as a function of strain rate and temperature. Also, the sugar crystal and the HMX crystal are both monoclinic, so they are similar microscopically as well. Both the PBS 9501 and the PBX 9501 have the same polymeric binder system. A micrograph of the PBX 9501 high explosive is shown in Fig. 1. Note that the HMX crystal has a very wide range of spectrum in sizes and the average diameter is about 100 μm.

PBX 9501 High Explosive

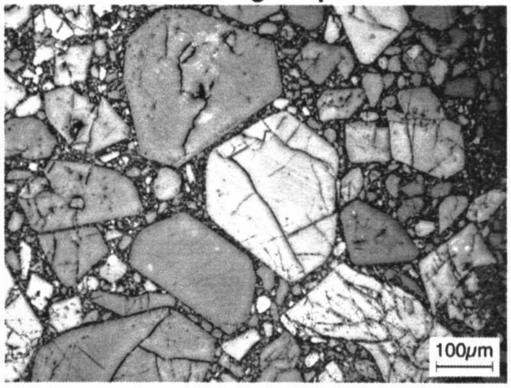


Figure 1: Micrograph of the PBX 9501 high explosive (courtesy of Cary Skidmore of Los Alamos National Laboratory).

The PBS 9501 simulant material is composed of 94 wt% C&H granulated sugar, 3.0 wt% estane, and 3.0 wt% nitroplasticizer, respectively. In making the PBS 9501 high explosive simulant material, estane (Estane 5703 from B.F.Goodrich) was first dissolved in 1,2-dichloroethane. This process took about 24 hours at room temperature during which gentle stirring was required. Then the nitroplasticizer was added and mixed with the desolved estane till the mixture was homogeneous. The C&H granulated sugar was added to the estane/nitroplasticizer mixture and was stirred by hand so that the sugar crystals were evenly coated. The solvent 1,2-dichloroethane was then evaporated in a hood and the mixture was stirred every several minutes by hand to prevent formation of a skin. The last traces of solvent were removed in a 60C° vacuum oven. Finally, the sugar mock was hydrostatically pressed at room temperature to the desired density and shape.

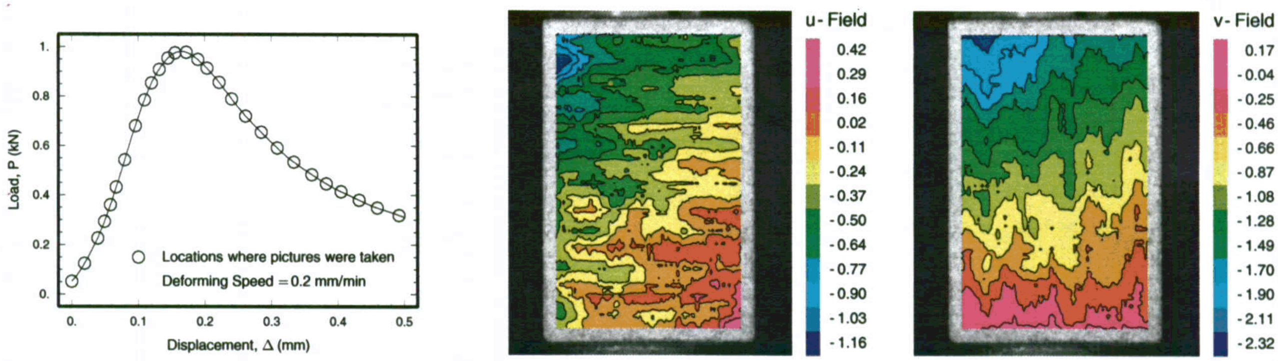
4 Experimental Measurement

We conducted two different experiments to investigate the nature of heterogeneity and to determine the minimum size of the representative element (RVE) size of the PBS 9501 high explosive simulant material. One experiment is the uniaxial compression and the other is thermal expansion.

4.1 Uniaxial compression experiment

The specimen we studied has a rectangular shape with the width of 12.7 mm and the thickness of 12.7 mm. The height of the specimen is 19.0 mm. We used a conventional INSTRON 1125 screw-driven loading frame to load the samples at a constant displacement rate of 0.2 mm/min, which is equivalent to a strain rate of $1.7 \times 10^{-4}\,\mathrm{sec}^{-1}$. Two plattens coated with Molykote spray were used in direct contact with the sample to ensure proper lubrication at both ends of the sample. A digital camera was setup in front of the sample to capture a series of images during the deformation process. The applied compressive load was continuously monitored during the test, and the variation of the applied load as a function of the displacement for the uniaxial compression test is shown in Fig. 2(a), where the circles represent the moments when the images of the specimen were taken. Using the digital image correlation technique described in the previous section, the deformation field within the compressive sample can be determined. In Fig. 2(b), the contour plots of the two displacement components are shown for the applied load $P = 400$ N.

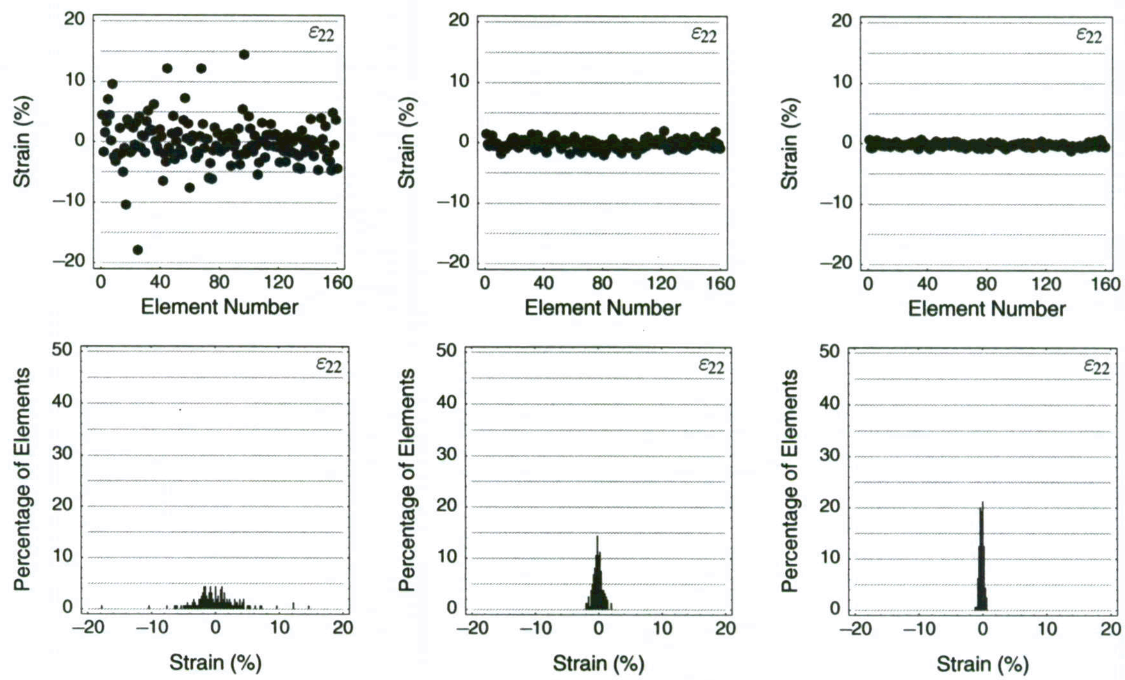
To determine the minimum size of the representative volume element of the heterogeneous material, we evaluated the strain distribution on the surface of the compressive sample based on the Eq. (6), which gives the average



(a) (b)

Figure 2: (a) Variation of applied load as a function of displacement in the uniaxial compression test; (b) Displacement field within the sample at the applied load $P = 400\,\text{N}$.

strain for a given material element $\mathbb{R}$. A matrix of 160 points were chosen on the sample surface and the digital image correlation calculations were carried out on those points. We also chose an image of the deformed sample at the early loading stage so that the deformation is in the elastic range and the strain measurement is not affected by damage or other deformation mechanisms due to applied load. As we have mentioned in the previous section, the deformation measurement using the DIC technique depends on the size of the small region or of the material element $\mathbb{R}$. In Fig. 3, the measurement results of the strain component along the loading direction, ϵ_{22}, are presented for three different sizes of material element $\mathbb{R}$ used in the correlation calculations. For each element size, the upper

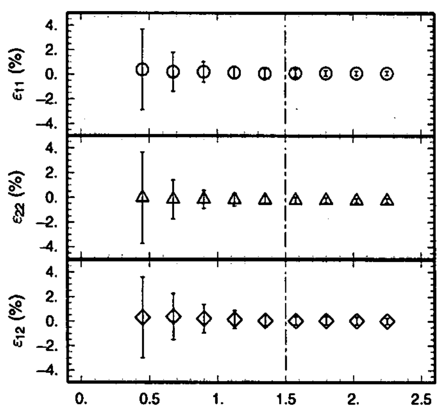


(a) (b) (c)

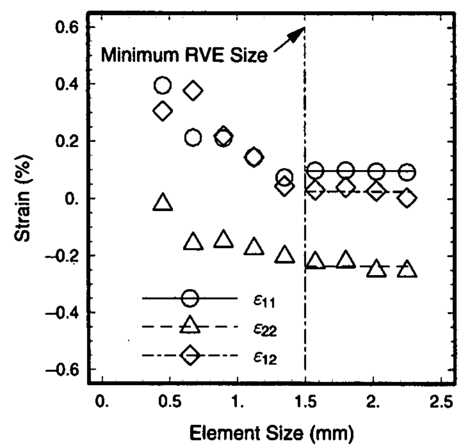
Figure 3: DIC results of the strain component along loading direction, ϵ_{22}, for different material element sizes: (a) 0.45 mm, (b) 0.90 mm, and (c) 1.35 mm.

plot in Fig. 3 shows the strain measurement at all the 160 points and the lower plot shows the histogram, which also resembles the distribution density of the measured strain of all the 160 elements. For small material element, the measured strain scatters over a wide range. As seen in Fig. 3(a), when the material element size is 0.45 mm, the component ϵ_{22} scatters from -18% to 15%, even though the element size is about 4 to 5 times of the average crystal diameter. As the size of the material element increases, the scatter of the measured strain decreases as shown in Figs. 3(b) and 3(c).

In Fig. 4(a), the mean values of all three in-plane strain components, together with their standard deviations, are presented as a function of different material element sizes ranging from 0.45 mm to 2.25 mm. One can see that the standard deviation is quite large for small material element and decreases rapidly as the material element size increases. For material elements larger than 1.5 mm, the standard deviation almost no longer changes. This stabilized standard deviation actually characterizes the uncertainties of the experimental technique itself and no longer represents the heterogeneous nature of the material. As a result, we may assign the length above which the heterogeneity does not affect the deformation measurement any more, as the minimum size of the representative volume element. An alternative way for determining the minimum RVE size is to look at the convergence of the mean value of the measured strain components. In Fig. 4(b), only the mean value of all three in-plane strain components is plotted against the size of the material elements. Once again, as we discussed in the previous section, for smaller material elements, the mean value of the measured strain changes rapidly and this is the case for all three in-plane strain components obtained using the digital image correlation technique. However, for material elements larger than 1.5 mm, each of the all three in-plane strain components converges to a constant. Moreover, the strain component along the loading direction, ϵ_{22}, actually converges to the value of the strain imposed from the boundary condition of the compressive sample. Therefore, we can conclude that the minimum size of the representative volume element for the heterogeneous PBS 9501, is approximately 1.5 mm.



(a)

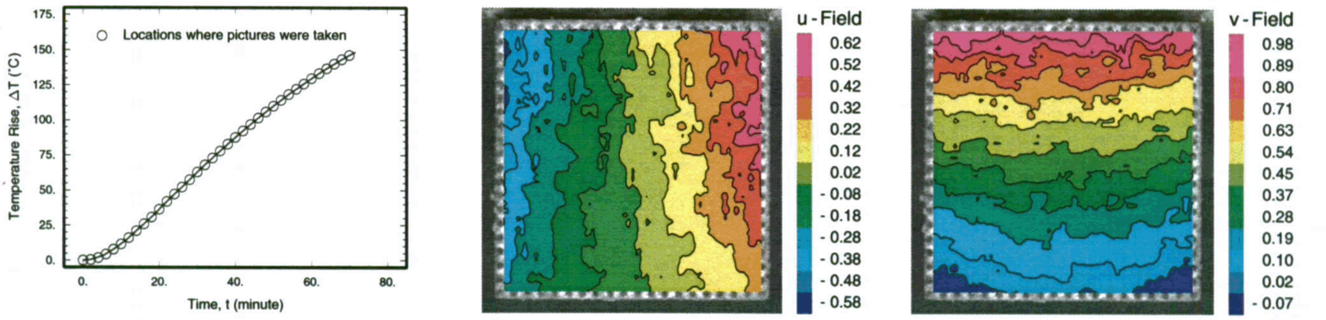


(b)

Figure 4: (a) Variation of the mean value and the standard deviation (as error bars) of measured strain as a function of material element size; (b) convergence of the strain component when material element size increases.

4.2 Thermal expansion experiment

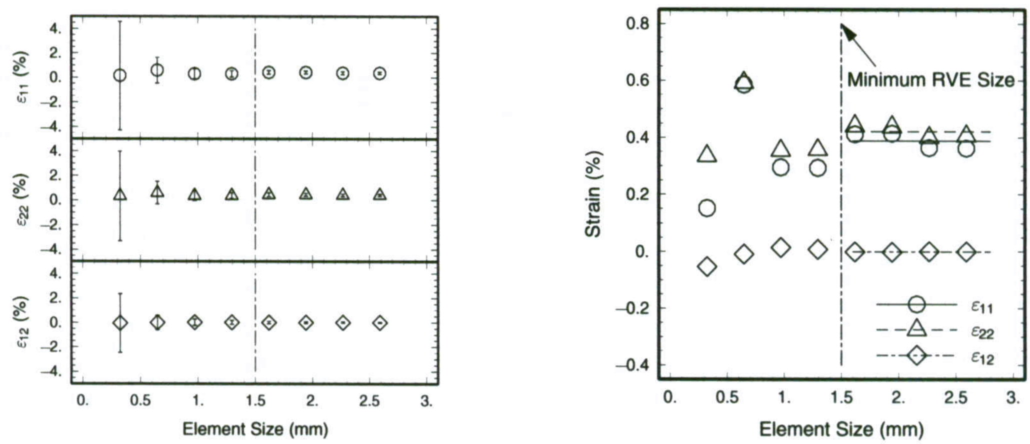
We also conducted experiment to investigate the expansion of a PBS 9501 sample due to uniform slow heating. The sample has the shape of a cube with 12.7 mm on each side. For applying the digital image correlation technique, we use a black paint to generate a random speckle pattern on one of the surfaces of the sample. The paint is the Krylon (more info here) that can withstand temperature up to 650°C (1200°F). We use a 500W Precision Vacuum Oven Model 19, which has a temperature range from room temperature to 200°C. Inside the oven an aluminum frame was used to elevate the sample and the PBS 9501 sample was placed on a piece of ceramic fire brick, which was sitting on top of the aluminum frame. Two thermocouples were attached to the sample via high temperature adhesive tape. One thermal couple is located near the top of the sample and the other near the bottom of the sample. We heat the sample by setting the power of the oven at maximum and it took about one hour for the temperature to rise from room temperature to 195°C. Typical temperature profile from the thermocouple is shown in Fig. fig:thermal-temperature-profile-expansion-displacement-field(a). A digital camera is set up in front of the oven to record the speckle image during the heating process. Figure 5(b) shows the contour plots of the two displacement components for the the moment when temperature rise $\Delta T = 83°C$. The average strain for different material element sizes is also calculated using the digital image correlation technnique, and the results are presented in Fig. 6. The overall



(a) (b)

Figure 5: (a) Variation of temperature as a function of time; (b) Displacement field within the sample at $\Delta T = 83°\text{C}$.

trend of the variation of the average strains as a function of the material element size is similar to that obtained in uniaxial compression experiment.



(a) (b)

Figure 6: (a) Variation of the mean value and the standard deviation (as error bars) of measured strain as a function of material element size, and (b) convergence of the strain component when material element size increases.

5 Concluding Remarks

In this study, we investigated experimentally the minimum size of the representative volume element of the heterogeneous material PBS 9501, a simulant of the PBX 9501 high explosive. Using the digital image correlation technique, we were able to determine that the minimum RVE size of the PBS 9501 is approximately 1.5 mm. This length is about 15 times of the average diameter of the crystals of the material. In a two-dimensional region, an RVE would include at least 250 crystals assuming that all the crystals have the same size as the average diameter, so that the response of the element can represent the overall mechanical behavior of the PBS 9501. This result is consistent with the observation of other numerical studies. For example, Elvin [9] studied the number of grains required to represent the homogeneous elastic behavior of polycrystalline ice. He considered fresh water, columnar-grained ice with relatively uniform grain size. Elvin found that, in two dimensions, at least 230 grains are needed to homogenize the elastic properties. He also found that the sliding condition along grain boundaries would influence the RVE size. In another numerical study, Ren and Zheng (2002) obtained the minimum RVE sizes for more than 500 kinds of cubic polycrystalline materials. Once again, they assumed that all the crystals have the same size, so that only the effect of crystal orientations was considered. They concluded that the minimum RVE size is about 20 times of the crystal size, which translates into that for a two-dimensional RVE, there are about 400 crystals in it. As can be seen in Fig. 1, the material we considered in this investigation is a lot more complicated than those considered in numerical studies. Meanwhile, even though we only measured the in-plane strain field, the deformation in the third direction definitely also affects the determination of the minimum RVE size in our experimental study.

We also need to point out that the minimum RVE size not only is material dependent, but also is material-property dependent. As proved by Nye [10], that the linear thermal conductivity of any cubic crystal is always isotropic, but the linear elasticity is anisotropic. As a result, for cubic polycrystal, the minimum RVE size for linear conductivity might be different from that for linear elasticity. Since we based our minimum RVE size determination on measuring deformation of the material under externally applied mechanical load, the minimum RVE size we obtained in this study is associated with the mechanical response of the material. Moreover, since we concentrated on the early stage of loading, where deformation is small, the minimum RVE size is ultimately related to the elastic behavior of the material.

Acknowledgments

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